APPENDIX B:

**MODELING GROUNDWATER IMPACTS FROM
THE PCB CAPACITOR LANDFILL**

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B.1 INTRODUCTION

As discussed in the Action Memorandum (Bainer and Berg 1998), 112 capacitors containing polychlorinated biphenyls (PCBs) were unearthed at the NIF construction site located in the northeastern portion of the Livermore Site (Figures B.1 and B.2). The capacitors and about 694 metric tons (766 short tons) of PCB-contaminated soils were removed. An excavated trench about 6.1 m (20 ft) wide, 21 m (70 ft) long and 5.2 m (17 ft) deep was used for this removal operation. The highest concentration of PCBs in the removed soils was 66 ppm. After removal, residual PCB levels were less than 1 ppm, consistent with environmental regulations and cleanup levels established in coordination with the CERCLA Remedial Project Managers (RPMs), who represent the U.S. Environmental Protection Agency (EPA), the California Department of Toxic Substances Control, and the San Francisco Bay Region Water Quality Board. The purpose of this appendix is to estimate the effects of PCBs on groundwater beneath the extraction trench.

B.2 PHYSICAL PROPERTIES OF PCBs

To perform any analyses for the extraction trench, physical and chemical properties of the capacitor material is needed. As mentioned in the Action Memorandum (Bainer and Berg 1998), the material in the capacitors was identified as Diaclor, although soil analyses from around the capacitors was reported as Aroclor 1254. PCBs were sold under the trade name Aroclor, although companies that used PCBs in the manufacture of capacitors often used other trade names, such as Diaclor. PCBs are produced by the chlorination of biphenyl. One to 10 hydrogen atoms of biphenyl can be replaced with chlorine atoms. Given all of the possible arrangements of chlorine atoms, there are 209 compounds (congeners) that are classified as PCBs (Mackay et al. 1992). These compounds do not readily degrade in groundwater systems.

Commercial mixtures of PCBs were manufactured under the trade name Aroclor. Aroclors 1260, 1254, and 1242 were most frequently used in electrical equipment. Aroclor 1260 contains 60% by weight chlorine, Aroclor 1254 contains 54% by weight chlorine, etc. For the purposes of this appendix, the capacitor material will be assumed to have the properties of the Aroclor 1254, and the results of surveys were reported as Aroclor 1254.

For the following calculations, two properties are required. The first is the solubility of the Aroclor in water. The Aroclor with the highest solubility would contribute the most material
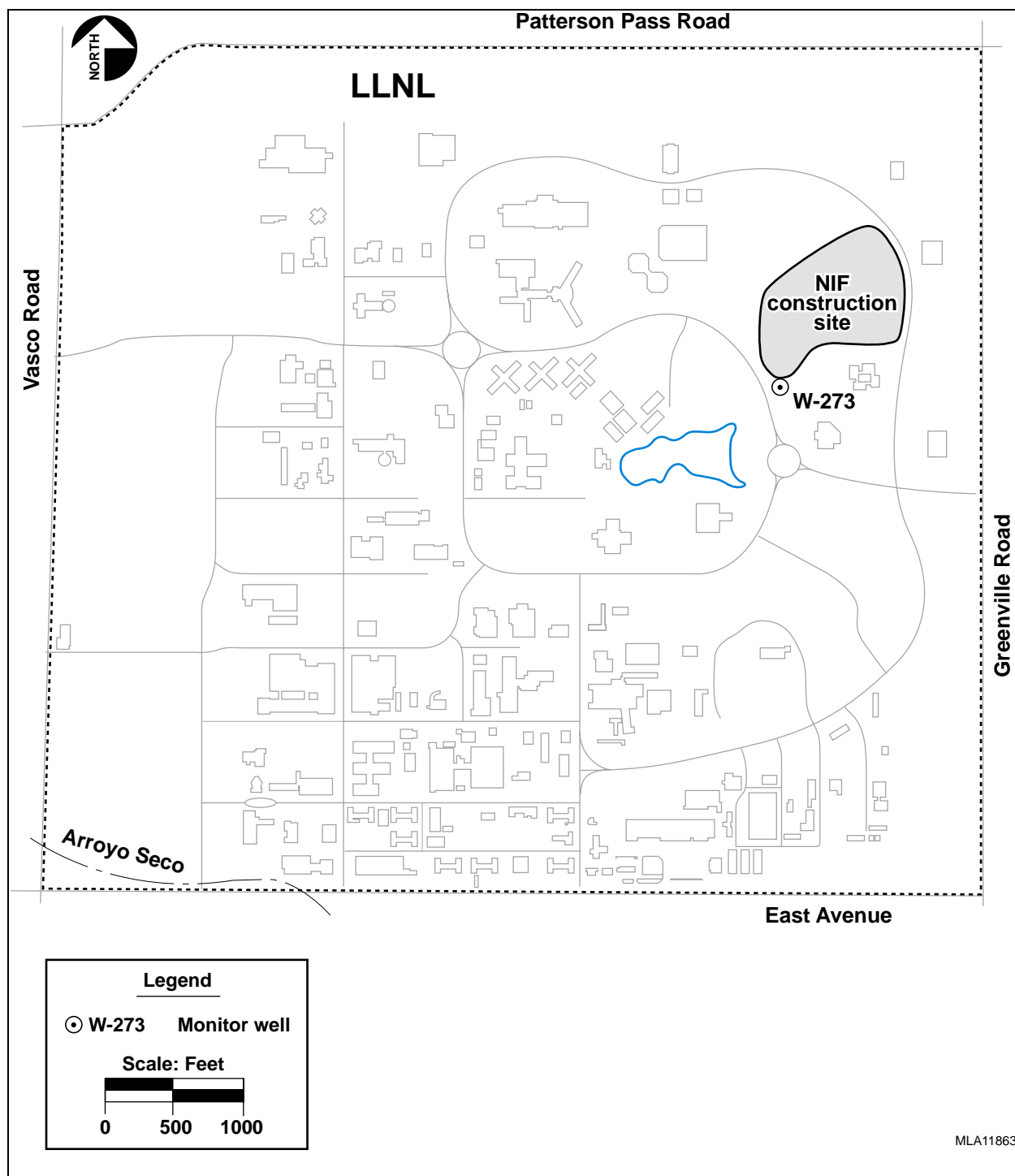
**FIGURE B.1 Location of the NIF Construction Site at the LLNL Livermore Site
(Source: Bainer and Berg 1998)**
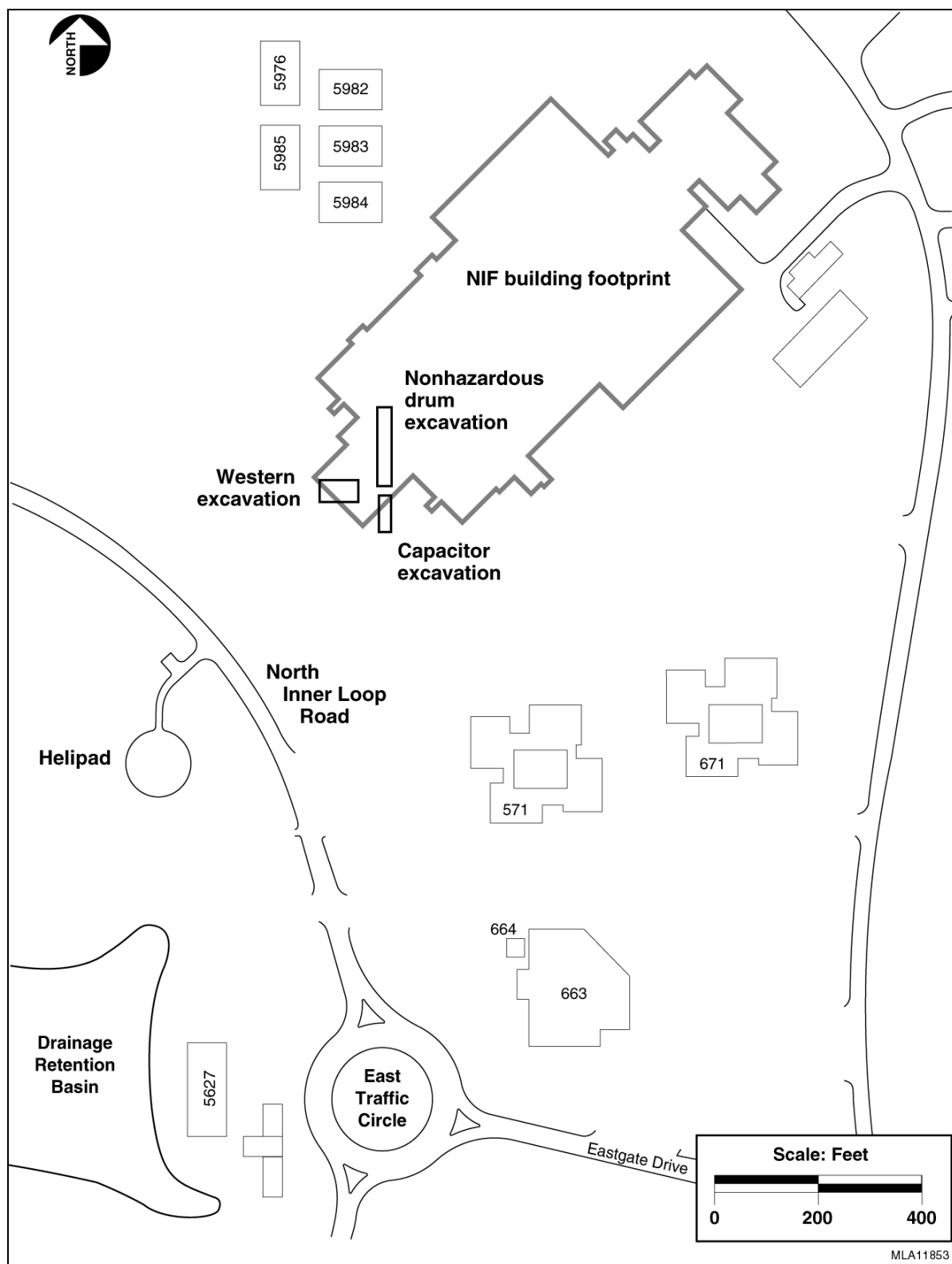
FIGURE B.2 Location of the Capacitor, Drum, and Western Excavations at the NIF Construction Area and Location of the East Traffic Circle Area (Source: Modified from Bainer and Berg 1998)

to the liquid phase and produce the greatest impact on the groundwater. The second property of interest is the partition coefficient (designated K_d) for the Aroclor. The partition coefficient defines the amount of material that would be in equilibrium between the sorbed and aqueous phase. That is, K_d is the mass of solute on the solid phase per unit mass of solid phase divided by the concentration of solute in solution (Freeze and Cherry 1979). When appropriately combined with soil properties, the distribution coefficient will provide an indication of how fast, relative to the groundwater velocity, the contaminant will move in the system. The higher the value of K_d, the slower the contaminant will move. Values for K_d are rarely available; however, a counterpart, K_{oc}, is available in the literature, where K_{oc} is the sorption coefficient normalized for organic carbon. K_d can be readily found given K_{oc} by using the following relation:

$$K_d = f_{oc} K_{oc} \,, \tag{B.1}$$

where f_{oc} is the fraction of organic material present in the soil. Table B.1 lists the solubilities and K_{oc} values from Montgomery and Welkom (1991). Of the potential Aroclors, 1242, with its high solubility and low K_{oc}, would produce the largest impacts to groundwater, and will, therefore, be used in the subsequent analyses.

B.3 FATE AND TRANSPORT

In its simplest form, contaminant transport through a porous material can be described by the following one-dimensional partial differential equation (Freeze and Cherry 1979):

$$\frac{\partial C}{\partial t} = -\frac{V}{R}\frac{\partial C}{\partial Z} + \frac{D}{R}\frac{\partial^2 C}{\partial Z^2} \,, \tag{B.2}$$

where:

C = contaminant concentration at time, t, depth Z;

D = dispersion coefficient;

R = retardation coefficient given by the expression $R = 1\ \rho_b K_d/\phi$, where ρ_b is the bulk density of the porous material and ϕ is its effective porosity;

t = time;

V = actual groundwater velocity; and

Z = vertical distance.

TABLE B.1 Aroclor Properties

Aroclor	Solubility (mg/L)	log K_{OC}	K_{OC} (mL/g)
1242	0.1	3.71	5,129
1254	0.057	5.61	407,400
1260	0.08	6.42	2,630,000

Source: Montgomery and Welkom (1991).

The dispersion coefficient, *D*, in Equation B.2 is assumed to follow the function form given by Bear (1972):

$$D = \alpha V \ , \tag{B.3}$$

where α is the dispersivity of the medium. Diffusional effects are assumed to be negligible relative to advection.

Dispersivity in Equation B.3 is assumed to be scale-dependent (Lallemand-Barres and Peaudecerf 1978); that is:

$$\alpha = 0.1L, \tag{B.4}$$

where *L* is distance from the top of the soil column to the water table.

Use of Equation B.2 makes the following simplifying approximations:

- Lateral transport from the surface to the water table is small (most infiltration occurs vertically),

- The infiltration velocity is constant in time and space, approximate for scoping calculations where the distance between the soil surface and groundwater surface is long,

- The soil is homogeneous,

- The contaminant is conservative (i.e., it does not decay or degrade in any way along its flow path),

- Sorption processes can be represented with a linear isotherm (i.e., sorption processes are fast and reversible).

If the impacts calculated with the model described by Equation B.2 are large, additional, more detailed calculations would be required in accordance with NEPA guidance.

In order to solve Equation B.2, two boundary conditions are needed. The first assumes that the concentration of the Aroclor goes to zero as the vertical distance goes to infinity. The second boundary condition is applied at the ground surface ($Z = 0.0$). At this location, the Aroclor is assumed to behave as a unit square-wave source in time. That is, the concentration at $Z = 0$ is some initial value, C_0, and remains so until a time equal to Δt, when the concentration returns to zero. The initial concentration is simply equal to the solubility of Aroclor. This type of boundary can be described by the following equation:

$$\frac{C}{C_0} = U(t - 0.0) - U(t - \Delta t) \,, \tag{B.5}$$

where U is the unit function (Kreyszig 1967).

Equation B.2, subject to the above boundary conditions, was solved using the method of Laplace transforms. The solution is given by the following expression (Tomasko 1992):

$$\frac{C}{C_0} = \frac{1}{2}(\text{erfc}(\frac{ZR - Vt}{2\sqrt{DRt}}) + e^{\frac{vz}{d}} \text{erfc}(\frac{ZR + Vt}{2\sqrt{DRt}}))$$

$$\tag{B.6}$$

$$- \frac{1}{2}H(t - \Delta t)(\text{erfc}(\frac{ZR - V(t - \Delta t)}{2\sqrt{DR(t - \Delta T)}}) + e^{\frac{VZ}{D}} \text{erfc}(\frac{ZR + V(t - \Delta t)}{2\sqrt{DR(t - \Delta t)}})) \,,$$

where H is the Heaviside function (Hildebrand 1976) such that:

$H(t - \Delta t) = 0$ for $t < \Delta t$,

and

$H(t - \Delta t) = 1$ for $t \geq \Delta t$, and

$$\text{erf}(\gamma) = 1 - \text{erf}(\gamma) = 1 - \frac{2}{\sqrt{\pi}} \int_{o}^{y} e^{-\lambda^2} d\lambda \,. \tag{B.7}$$

B.4 POROUS MEDIUM INPUT VALUES

To solve Equation B.6, a number of physical parameters are required. Many of these were discussed in the main text. The vertical distance from the ground surface to the water table is 13 m (43 ft) for a water table at a depth of 18 m (60 ft), and an excavation depth of 5.2 m (17 ft) for the capacitor trench. Retardation, R, for Aroclor 1242 is about 487 using a fraction of organic carbon in the soil of 1.7% (Maidment 1992), an average bulk density for the soil of 1.89 g/cm^3, and an average effective porosity of 0.339 derived from soil sample data at the NIF site (Stephens and Associates, Inc. 1996). The vertical groundwater velocity is assumed to be equal to the average annual recharge to HSU 1, 33 mm/yr (1.33 in./yr [0.11 ft/yr]) (Vogele et al. 1996). For this velocity and travel distance, the computed dispersion coefficient is 0.04 m^2/yr (0.47 ft^2/yr).

In addition to the above parameters, the duration of the Aroclor 1242 is needed for Equation B.6. This duration can be roughly approximated by assuming that the infiltrating precipitation dissolves the PCB from the soil at a solubility-limited concentration and then transports the solute vertically downwards to the water table. By mass conservation,

$$\Delta t = \frac{\rho_{1242} t_h}{V Sol},$$
(B.8)

where:

Sol = solubility of the Aroclor,

t = thickness of the residual contamination (about 0.3 m [1 ft]), and

ρ_{1242} = density of Aroclor 1242.

As specified in the Action Memorandum (Bainer and Berg 1998), the PCBs were cleaned up to a concentration of less than 1 ppm. For the soils at the NIF site (Stephens and Associates, Inc. 1996), the average dry density is about 1.75 g/cm^3, and, therefore, the concentration of Aroclor is 1.75×10^{-6} g/cm^3. The duration of residual Aroclor in the soil is thus about 160 years.

B.5 CALCULATIONS

Figure B.3 shows the normalized concentration (C/C$_0$) as a function of time (break-through curve) calculated with Equation B.6 and as many site-specific parameters as possible. For these conditions, Aroclor 1242 will attain a maximum concentration of about 0.001 after
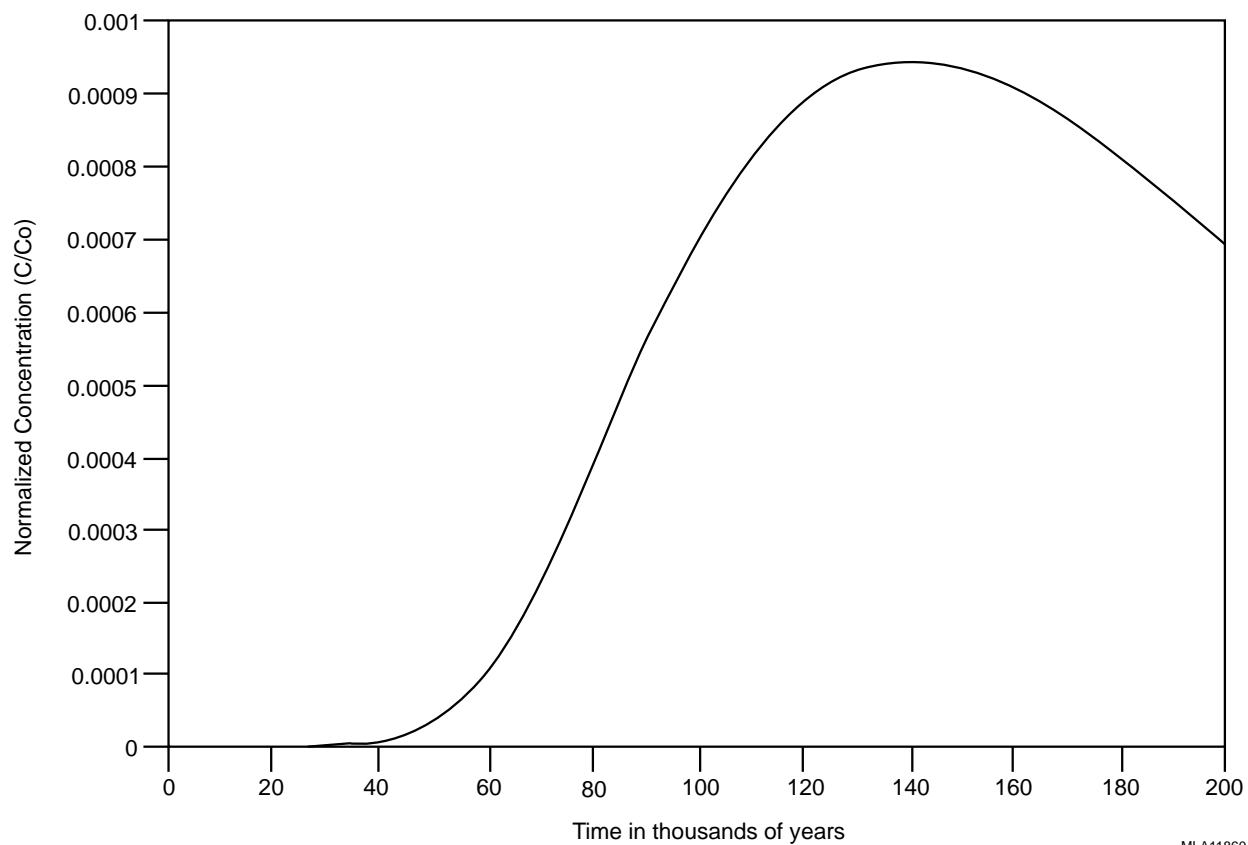
FIGURE B.3 Water Table Breakthrough Curve for PCB (Aroclor 1242) at the NIF Construction Area

approximately 140,000 years. This long breakthrough curve is primarily the result of the high degree of retardation and is not unexpected. To get an actual water concentration at the water table, the value 0.001 must be multiplied by the initial concentration at the ground surface (assumed to be equal to the solubility of Aroclor 1242 — 1.0×10^{-7} g/cm^3). The resulting maximum Aroclor concentration at the water table would, therefore, be about 1.0×10^{-10} g/cm^3. This value is about 20% of the EPA maximum contaminant level (MCL) for drinking water (EPA 1994).

Once the infiltrating water that contains Aroclor 1242 reaches the water table, mixing will occur. A simple mixing model (Tomasko 1992) was used, as found from the following expression:

$$d_f = \frac{V_d t_h}{I \, X_l \, \phi} + 1 , \tag{B.9}$$

where:

     I = infiltration rate,

     t_h = thickness of HSU 1 (9 m [30 ft]),

     V_d = Darcy velocity in HSU 1 (about 0.34 m/yr [1.1 ft/yr]), and

     X_l = width of contamination zone parallel to the direction of groundwater flow (assumed to be equal to the width of the excavation trench — 6 m [20 ft]).

The concentration of Aroclor 1242 in groundwater after mixing would, therefore, be about 2.5×10^{-12} g/cm^3 (0.0025 ppb), which is about 0.5% of the MCL for drinking water.

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